

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
26 May 2005 (26.05.2005)

PCT

(10) International Publication Number
WO 2005/047520 A3

(51) International Patent Classification⁷: **G06F 19/00**

(21) International Application Number:
PCT/US2004/037291

(22) International Filing Date:
8 November 2004 (08.11.2004)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/518,220 7 November 2003 (07.11.2003) US

(71) Applicant (*for all designated States except US*): **DNA SOFTWARE, INC.** [US/US]; 120-1/2 West Washington Street, Ann Arbor, MI 48108 (US).

(72) Inventors; and

(75) Inventors/Applicants (*for US only*): **SANTALUCIA, John** [US/US]; 563 North Rosedale Court, Grosse Pointe Woods, MI 48236 (US). **HICKS, Donald, A.** [US/US]; 233 Hunters Trail, Ann Arbor, MI 48103 (US). **SARO, Pirro** [AL/US]; 66 Orange Street, Apt. 504, New Haven, CT 06510 (US).

(74) Agents: **BROW, Mary, Ann, D.** et al.; Medlen & Carroll, LLP, 101 Howard Street, Suite 350, San Francisco, CA 94105 (US).

(81) Designated States (*unless otherwise indicated, for every kind of national protection available*): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (*unless otherwise indicated, for every kind of regional protection available*): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

— with international search report

(88) Date of publication of the international search report:
6 October 2005

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: **SYSTEM AND METHODS FOR THREE DIMENSIONAL MOLECULAR STRUCTURAL ANALYSIS**

(57) Abstract: The present invention relates to methods and systems for the accurate prediction of nucleic acid, e.g., RNA and DNA, and other macromolecular and biomolecular three-dimensional structure from sequence and constraint information.

WO 2005/047520 A3